

5-Ethyl-1-methyl-5-(1-phenylethyl)pyrimidine-2,4,6(1H,3H,5H)-trione
61346-87-0 | DTXSID60818264

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.09e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.53e-01

Confidence level: 3.69e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,2',3,4,4',5,5'- Heptachlorobiphenyl</div> <div>Measured: 3.75e-09</div> <div>Predicted: 1.07e-06</div>	<div>Image not found</div> <div>Decachlorobiphenyl</div> <div>Measured: 1.50e-09</div> <div>Predicted: 1.75e-07</div>	<div>Image not found</div> <div>4-tert-Butylcyclohexyl acetate</div> <div>Measured: 1.27e-05</div> <div>Predicted: 2.32e-02</div>
<div>Image not found</div> <div>Fenpicionil</div> <div>Measured: 7.50e-09</div> <div>Predicted: 3.72e-07</div>	<div>Image not found</div> <div>Oxadiargyl</div> <div>Measured: 3.00e-05</div> <div>Predicted: 1.54e-08</div>	